10568572

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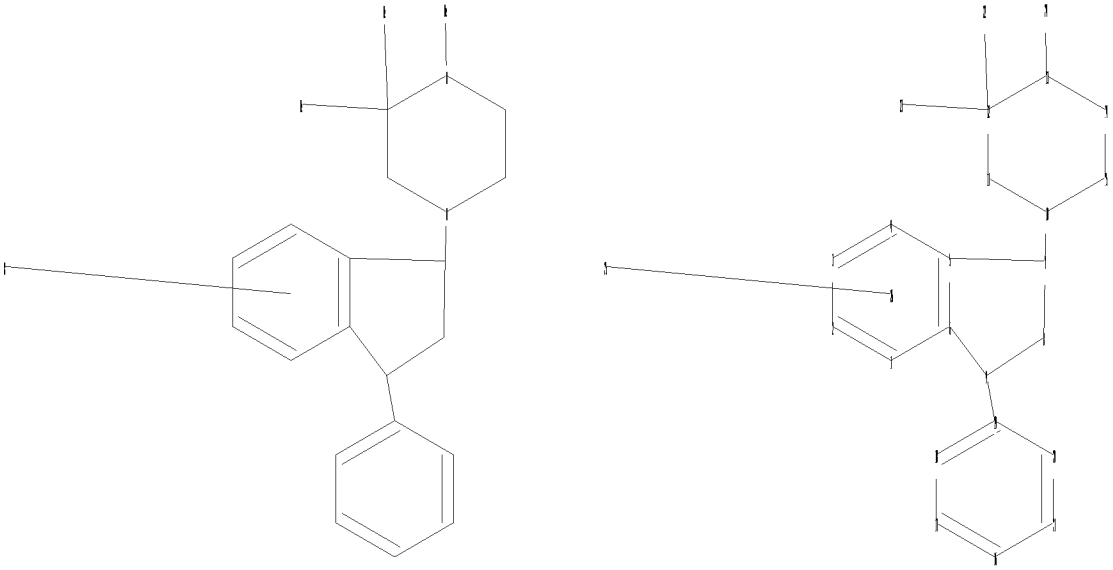

chain nodes :
22 23 24 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
chain bonds :
7-10 9-19 12-22 12-23 13-24
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
5-7 6-9 7-8 7-10 8-9 10-11 10-15 11-12 12-13 13-14 14-15
exact bonds :
9-19 12-22 12-23 13-24
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom

L1 STRUCTURE UPLOADED

=> s l1 sss full
FULL SEARCH INITIATED 19:43:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1334 TO ITERATE

100.0% PROCESSED 1334 ITERATIONS 43 ANSWERS

SEARCH TIME: 00.00.01

L2 43 SEA SSS FUL L1

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5510025 NC>1
L3 24 L2 AND NC>1

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 183.51 183.72

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FILE LAST UPDATED: 9 May 2008 (20080509/ED)

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=> s l3
L4 4 L3

=> d l4 1-4 bib abs hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:845375 CAPLUS
DN 145:271813
TI Process for making trans-1-((1R,3S)-6-chloro-3-phenylindan-1-yl)-3,3-dimethylpiperazine
IN Dahl, Allan, Carsten; Woehlk Nielsen, Christina; Suteu, Christina; Robin, David; Broesen, Peter
PA H. Lundbeck A/S, Den.
SO PCT Int. Appl., 39pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2006086984 A1 20060824 WO 2006-DK86 20060214
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
AU 2006215955 A1 20060824 AU 2006-215955 20060214
CA 2597615 A1 20060824 CA 2006-2597615 20060214
EP 1853574 A1 20071114 EP 2006-706057 20060214
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU
KR 2007103386 A 20071023 KR 2007-716237 20070716
MX 200709814 A 20070907 MX 2007-9814 20070814
IN 2007CN03582 A 20071116 IN 2007-CN3582 20070816
CN 101137632 A 20080305 CN 2006-80005207 20070816
NO 2007004642 A 20070912 NO 2007-4642 20070912
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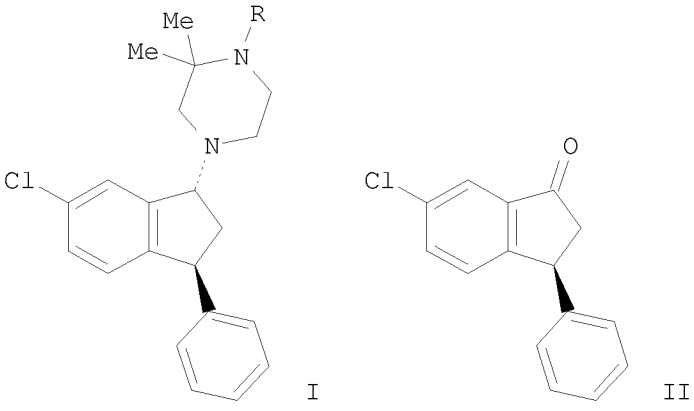
US 2005-653428P P 20050216
WO 2006-DK86 W 20060214
OS CASREACT 145:271813; MARPAT 145:271813
GI



AB Described is a method for making the trans-1-((1R,3S)-6-chloro-3-phenylindan-1-yl)-3,3-dimethylpiperazine (I; R = H) and salts thereof and a similar method for making 4-((1R,3S)-6-chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine (I; R = Me) and salts thereof, which method comprises conversion of a compound of formula II to the compound of formula I.

IT 170381-17-6P 846061-36-7P 846541-66-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for making trans-(chlorophenylindanyl)dimethylpiperazine)

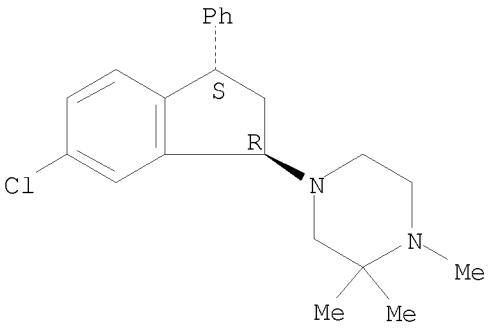
RN 170381-17-6 CAPLUS

CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(-)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

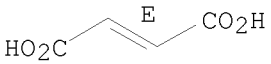
Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

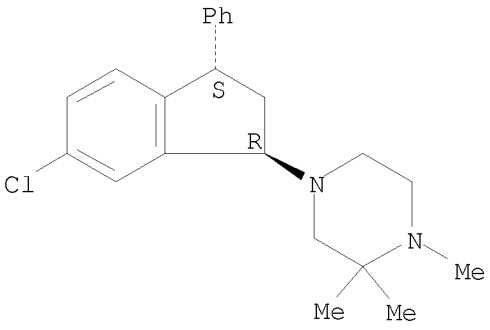


RN 846061-36-7 CAPLUS
CN Butanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:1) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-15-6
CMF C4 H6 O4

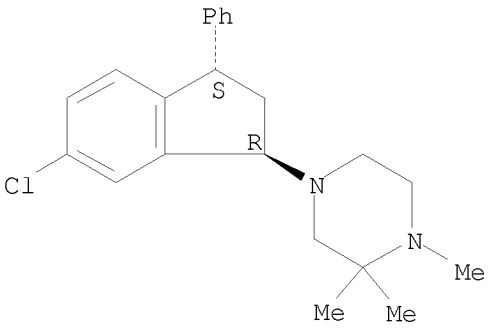
$HO_2C—CH_2—CH_2—CO_2H$

RN 846541-66-0 CAPLUS
CN Propanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:1) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 141-82-2
CMF C3 H4 O4

$HO_2C—CH_2—CO_2H$

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:158651 CAPLUS
DN 142:261558
TI Succinate and malonate salts of trans-4-(1R,3S)-6-chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine and their preparation, pharmaceutical compositions, and use as medicaments, particularly as antipsychotics
IN Lopez De Diego, Heidi; Nielsen, Ole; Ringgard, Lone Munch; Svane, Henrik; Dahl, Allan Carsten; Howells, Mark; Bang-Andersen, Benny
PA H. Lundbeck A/S, Den.
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005016900	A1	20050224	WO 2004-DK545	20040818
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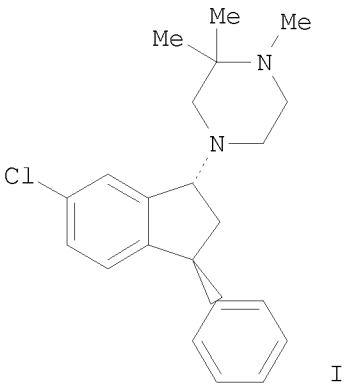
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004265021	A1	20050224	AU 2004-265021	20040818
	CA 2536144	A1	20050224	CA 2004-2536144	20040818
	EP 1658277	A1	20060524	EP 2004-762772	20040818
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	CN 1839124	A	20060927	CN 2004-80023725	20040818
	BR 2004013595	A	20061017	BR 2004-13595	20040818
	JP 2007502783	T	20070215	JP 2006-523528	20040818
	IN 2006CN00557	A	20070622	IN 2006-CN557	20060215
	MX 2006PA01838	A	20060504	MX 2006-PA1838	20060216
	NO 2006001151	A	20060310	NO 2006-1151	20060310
	US 20060281759	A1	20061214	US 2006-568572	20060814
PRAI	DK 2003-1180	A	20030818		
	US 2003-496058P	P	20030818		
	DK 2003-1305	A	20030911		
	US 2003-520246P	P	20031114		
	WO 2004-DK545	W	20040818		

OS CASREACT 142:261558; MARPAT 142:261558
GI



I

AB The salts 4-((1R,3S)-6-chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine (I) hydrogen succinate and hydrogen malonate are disclosed. Also disclosed are pharmaceutical compns. containing these salts, and their medical uses, including those for the treatment of schizophrenia and other psychotic disorders. Also described are methods for the preparation of I, and medical uses thereof. I, which has been previously described, is a mixed D1/D2 antagonist and a 5-HT2 antagonist, with an affinity for α1 adrenoceptors as well. The fumarate salt of I has also been described. The invention salts (hydrogen succinate and hydrogen malonate) show a considerably larger aqueous solubility than does the fumarate. The invention salts also show favorable stability and non-hygroscopicity. Two crystalline forms of the hydrogen succinate were observed The salts are expected to show the same general utility as I toward a variety of CNS disease states (no data). The 5-HT2 antagonistic activity of the salts suggest a relatively low risk of extrapyramidal side effects. For example, racemic cis-6-chloro-3-phenylindan-1-ol was resolved by chiral chromatog. or enzymic resolution to give the (+)-(1S,3S) isomer, which was chlorinated with SOCl2 and then aminated with 1,2,2-trimethylpiperazine, to give I as a cis/trans mixture Conversion of the ee base of I to the hydrogen fumarate salt by precipitation with fumaric acid gave I fumarate with no detectable cis isomer. This stereochem. pure salt was converted back to the ee base of I with aqueous NH3, followed by extraction into PhMe, evaporation, and conversion to the hydrogen succinate by precipitation om acetone. The initially formed succinate was the beta form, but repetitions of the procedure gave the more stable alpha form. In water at room temperature, I salts had the following solubilities: alpha (1:1) succinate 13, (1:1) malonate 15, and fumarate 1.5 mg/mL. The new salts, and particularly the succinate, showed better overall heat and light stability relative to the fumarate.

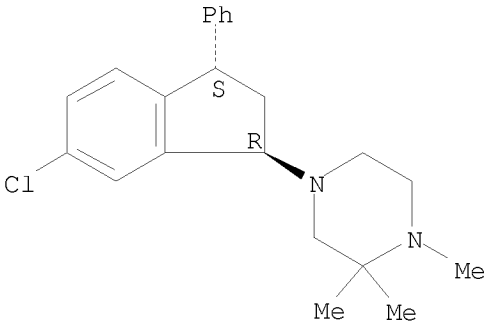
IT 846061-36-7P, (-)-trans-4-((1R,3S)-6-Chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine hydrogen succinate 846541-66-0P, trans-4-((1R,3S)-6-Chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine hydrogen malonate
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of succinate and malonate salts of (chlorophenylindanyl)trimethylpiperazine as antipsychotics)

RN 846061-36-7 CAPLUS
CN Butanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:1) (CA INDEX NAME)

CM 1

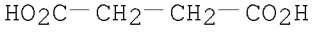
CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-15-6
CMF C4 H6 O4

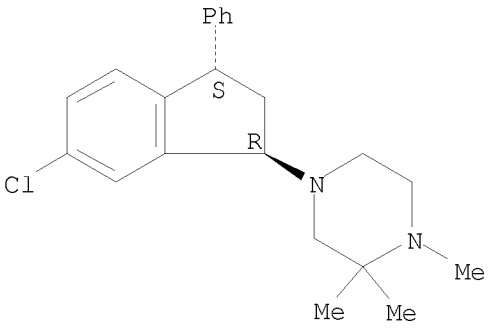


RN 846541-66-0 CAPLUS
CN Propanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:1) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 141-82-2
CMF C3 H4 O4

$HO_2C—CH_2—CO_2H$

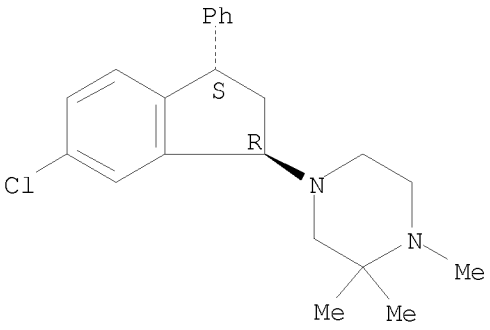
IT 846541-64-8P, trans-4-((1R,3S)-6-Chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine succinate 846541-65-9P, trans-4-((1R,3S)-6-Chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine malonate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of succinate and malonate salts of (chlorophenylindanyl)trimethylpiperazine as antipsychotics)

RN 846541-64-8 CAPLUS
CN Butanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:?) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-15-6
CMF C4 H6 O4

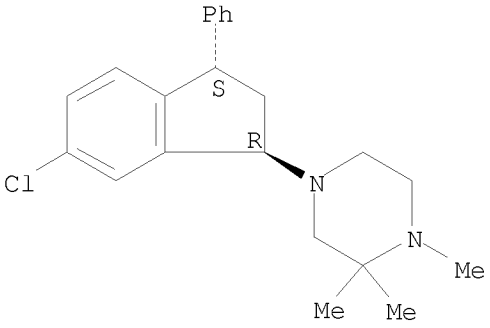
$HO_2C—CH_2—CH_2—CO_2H$

RN 846541-65-9 CAPLUS
CN Propanedioic acid, compd. with 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethylpiperazine (1:?) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 141-82-2
CMF C3 H4 O4

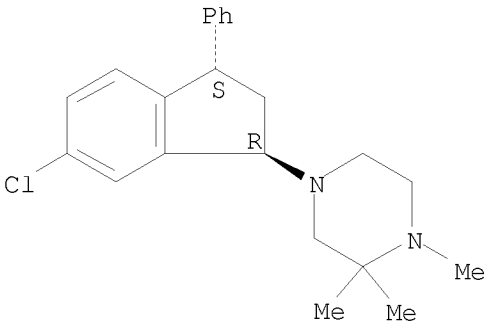
$HO_2C—CH_2—CO_2H$

IT 170381-17-6P, (-)-trans-4-((1R,3S)-6-Chloro-3-phenylindan-1-yl)-1,2,2-trimethylpiperazine hydrogen fumarate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of succinate and malonate salts of (chlorophenylindanyl)trimethylpiperazine as antipsychotics)
RN 170381-17-6 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(-)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

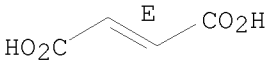
Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-17-8
CMF C4 H4 O4

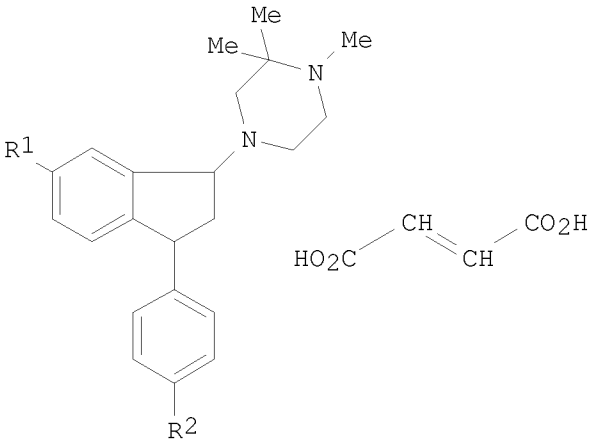
Double bond geometry as shown.



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of succinate and malonate salts of (chlorophenylindanyl)trimethylpiperazine as antipsychotics

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1995:849924 CAPLUS
DN 123:329244
TI Enhanced D1 Affinity in a Series of Piperazine Ring Substituted 1-Piperazino-3-Arylindans with Potential Atypical Antipsychotic Activity
AU Bogeso, Klaus P.; Arnt, Jorn; Frederiksen, Kristen; Hansen, Hans Otto; Hyttel, John; Pedersen, Henrik
CS Research Development H. Lundbeck A/S, Copenhagen, DK-2500, Den.
SO Journal of Medicinal Chemistry (1995), 38(22), 4380-92
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I R^1 = Cl, R^2 = H

II R^1 = F, R^2 = F

AB A study of the effect of aromatic substitution on D1 and D2 affinity in a series of previously reported trans-1-piperazino-3-phenylindans shows similar structure-activity relationships for the two receptor sites. 6-Substituted derivs. have affinity for both receptors, and 6-chloro- or 6-fluoro-substituted derivs. show preference for D1 receptors. D1 affinity and selectivity are significantly increased in a series of new piperazine ring substituted derivs. Potent D1 and D2 antagonism in vivo are confined to derivs. with relatively small substituents in the 2-position of the piperazine ring (e.g. 2-Me, 2,2-di-Me, 2-spirocyclobutyl or 2-spirocyclopentyl). Consequently, the effect of aromatic substitution is examined in a series of 1-(2,2-dimethylpiperazino)-3-arylindans. All these compds. except the 4-, 5-, 7- and 4'-chloro-substituted derivs. have potent D1 affinity (IC50's below 10 nM) and the majority of the compds. antagonize SK&F 38393-induced circling in 6-OHDA-lesioned rats with ED50 values about 1 μmol/kg. In vitro all compds. show preference for D1 receptors, but in vivo they are equally effective as D1 and D2 antagonists. The compds. have high affinity for 5-HT2 receptors and selected compds. show high affinity for α1-adrenoceptors. Furthermore, some of the tested compds. do not induce catalepsy in rats. These compds. have the potential of being "atypical" antipsychotics and have consequently been selected for further studies. The non-receptor-blocking enantiomers are shown to be inhibitors of DA and NE uptake in accordance with previous observations in compds. unsubstituted in the piperazine ring. Two compds., I and II, block DA uptake with IC50 values below 10 nM. Finally, the observed structure-activity relationships are discussed in relation to previously published pharmacophore models for D2 and 5-HT2 receptors. It is concluded that the piperazine substituents might induce a different binding mode at the dopamine receptor sites, perhaps only at the D1 receptor site.

IT 153626-89-2P 153627-01-1P 153627-62-4P
153627-64-6P 170381-17-6P 170381-19-8P
170381-25-6P 170381-27-8P 170381-29-0P
170381-36-9P 170381-37-0P 170381-39-2P

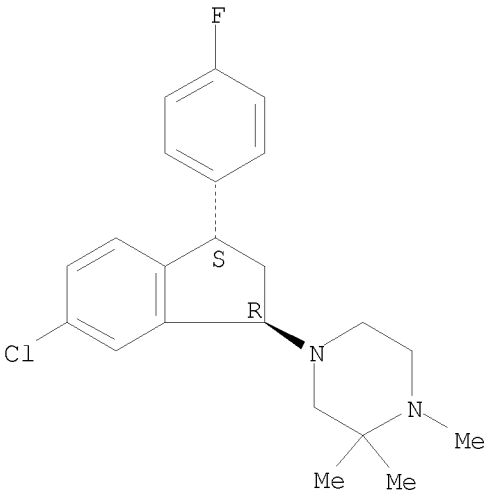
170381-45-0P 170381-48-3P 170381-50-7P
170381-52-9P 170381-54-1P 170381-56-3P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(structure activity relations in D1- and D2-dopaminergic receptor affinity of piperazinoarylindans)

RN 153626-89-2 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 153626-88-1
CMF C22 H26 Cl F N2

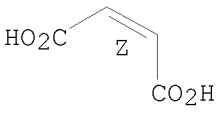
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

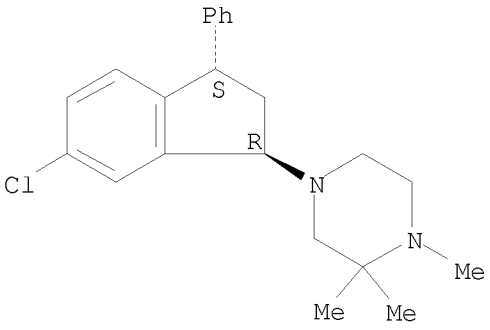


RN 153627-01-1 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 153627-00-0
CMF C22 H27 Cl N2

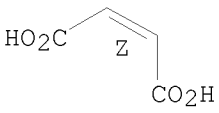
Relative stereochemistry.



CM 2

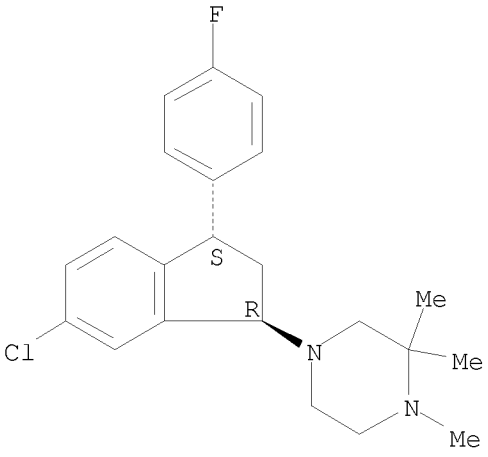
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 153627-62-4 CAPLUS
CN Piperazine, 4-[6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, dihydrochloride, trans-(-)- (9CI) (CA INDEX NAME)

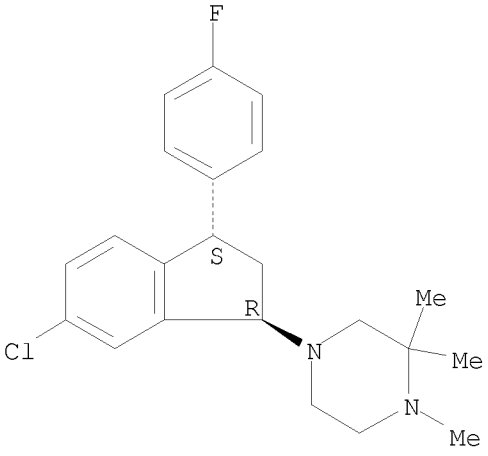
Rotation (-). Absolute stereochemistry unknown.



●2 HCl

RN 153627-64-6 CAPLUS
CN Piperazine, 4-[6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, dihydrochloride, trans-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



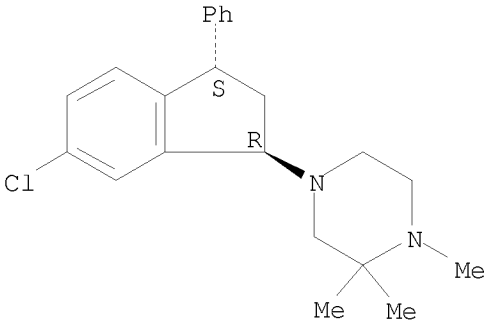
●2 HCl

RN 170381-17-6 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(-)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-16-5
CMF C22 H27 Cl N2

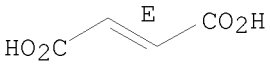
Absolute stereochemistry. Rotation (-).



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

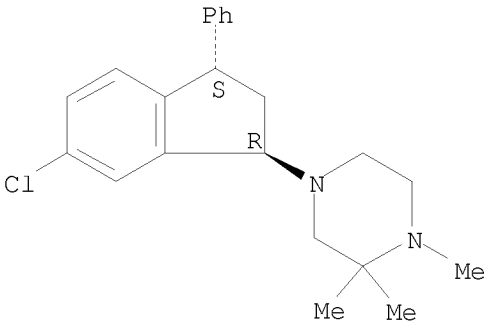


RN 170381-19-8 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(+)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-18-7
CMF C22 H27 Cl N2

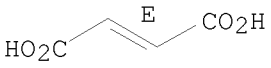
Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

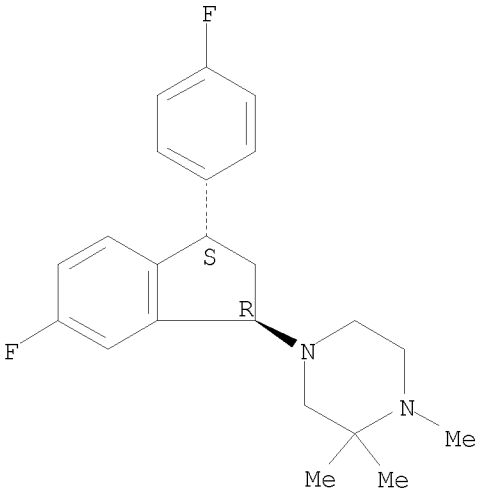


RN 170381-25-6 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-24-5
CMF C22 H26 F2 N2

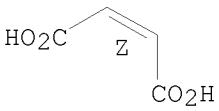
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



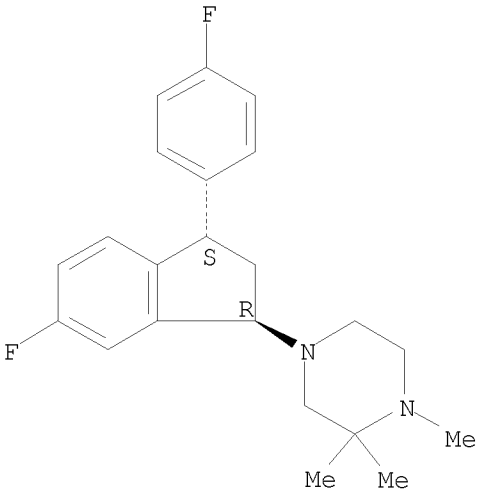
RN 170381-27-8 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(+)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX

NAME)

CM 1

CRN 170381-26-7
CMF C22 H26 F2 N2

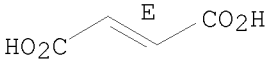
Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

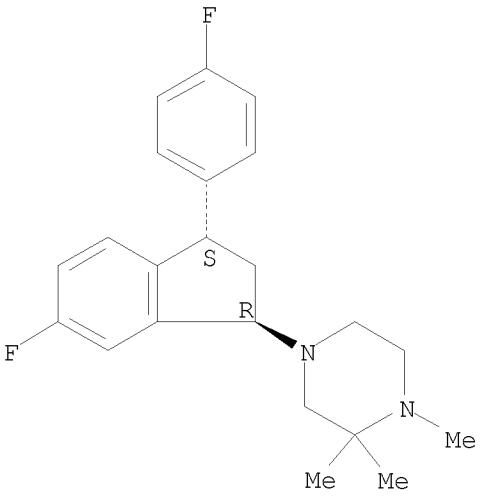


RN 170381-29-0 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(-)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-28-9
CMF C22 H26 F2 N2

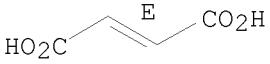
Rotation (-). Absolute stereochemistry unknown.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

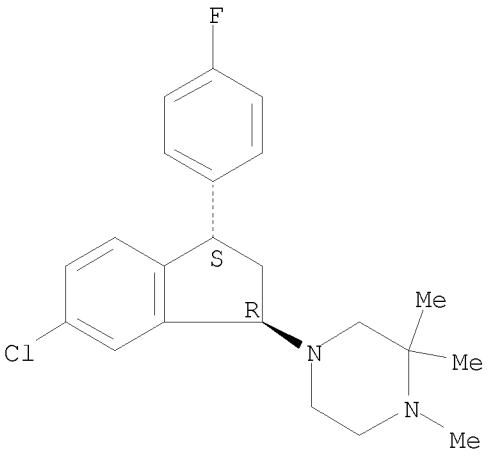


RN 170381-36-9 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(+)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 153627-65-7
CMF C22 H26 Cl F N2

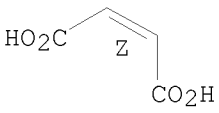
Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

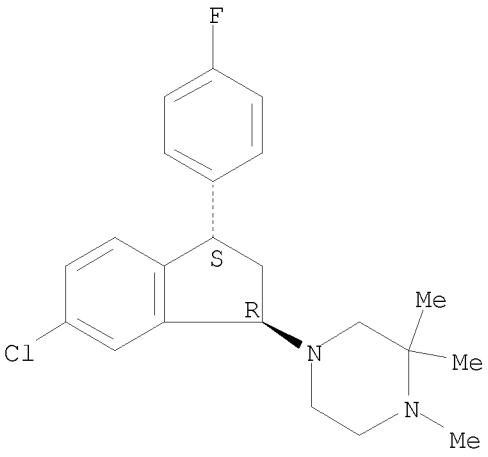


RN 170381-37-0 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-(-)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 153627-63-5
CMF C22 H26 Cl F N2

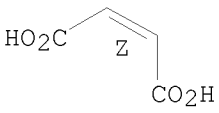
Rotation (-). Absolute stereochemistry unknown.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

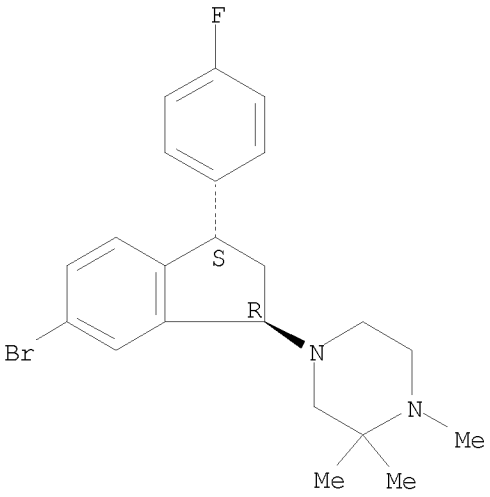


RN 170381-39-2 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-bromo-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-38-1
CMF C22 H26 Br F N2

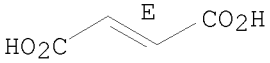
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

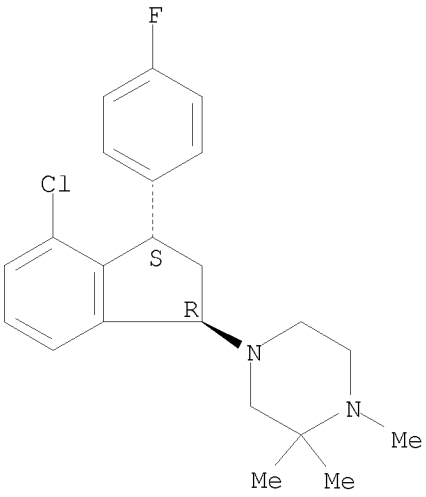


RN 170381-45-0 CAPLUS
CN Piperazine, 4-[4-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:2), trans- (9CI) (CA INDEX NAME)

CM 1

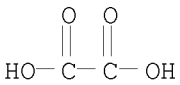
CRN 170381-44-9
CMF C22 H26 Cl F N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

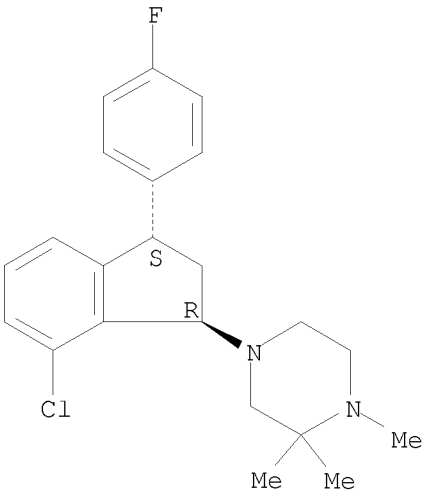


RN 170381-48-3 CAPLUS
CN Piperazine, 4-[7-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

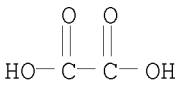
CRN 170381-47-2
CMF C22 H26 Cl F N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

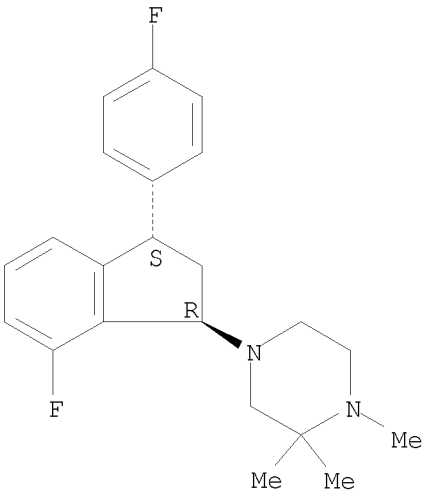


RN 170381-50-7 CAPLUS
CN Piperazine, 4-[7-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

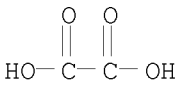
CRN 170381-49-4
CMF C22 H26 F2 N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

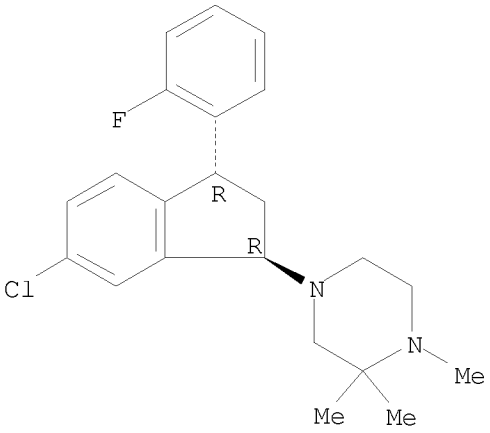


RN 170381-52-9 CAPLUS
CN Piperazine, 4-[(1R,3R)-6-chloro-3-(2-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-51-8
CMF C22 H26 Cl F N2

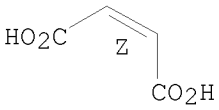
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

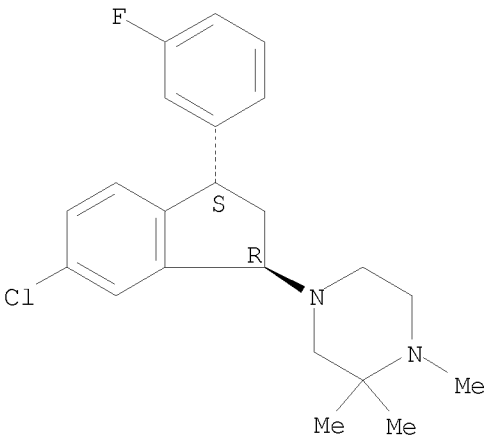


RN 170381-54-1 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(3-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-53-0
CMF C22 H26 Cl F N2

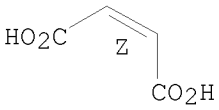
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

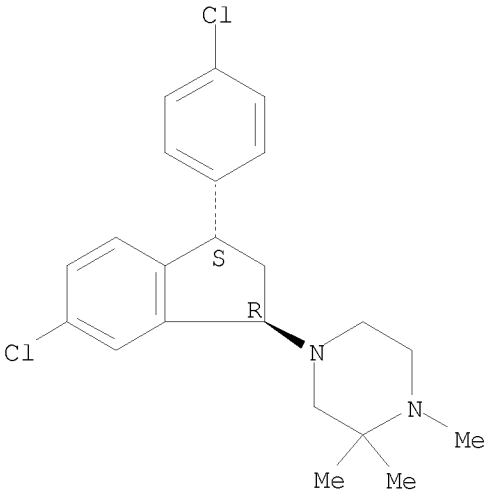


RN 170381-56-3 CAPLUS
CN Piperazine, 4-[6-chloro-3-(4-chlorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

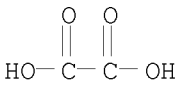
CRN 170381-55-2
CMF C22 H26 Cl2 N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:191735 CAPLUS
DN 120:191735
OREF 120:33943a,33946a
TI 1-piperazino-1,2-dihydroindene derivatives
IN Boegesoe, Klaus; Bregnedal, Peter
PA Lundbeck, H. a/s, Den.
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9322293	A1	19931111	WO 1993-DK136	19930423
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	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	ZA 9302840	A	19931123	ZA 1993-2840	19930422
	AU 9340599	A	19931129	AU 1993-40599	19930423
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	EP 638073	A1	19950215	EP 1993-909807	19930423
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	CZ 281676	B6	19961211	CZ 1994-2619	19930423
	RU 2114106	C1	19980627	RU 1994-45948	19930423
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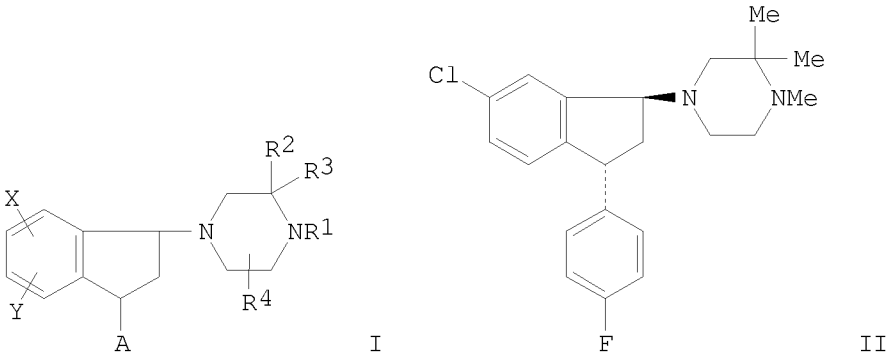
OS MARPAT 120:191735

GI



I II

AB Trans-isomers of 1-piperazino-1,2-dihydroindene compds. having general formula I (R1-R4 = H, alkyl, etc.; X, Y = H, halo, etc.; A = Ph, etc.) and their uses as potential antagonists of D1 receptors are claimed. The compds. are useful in the treatment of diseases in the central nervous system, in particular psychosis, schizophrenia (pos. as well as neg. symptoms), anxiety, depression, sleep disturbances, migraine, Parkinson's disease or cocaine abuse. An example compound, (±)-trans-4-[6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-dimethylpiperazine (II) was prepared The activity of II as D1, D2 and 5-HT2 receptor antagonists was tested.

IT 153626-89-2 153626-99-4 153627-01-1
153627-13-5 153627-62-4 153627-64-6
170381-25-6 170381-39-2 170381-45-0

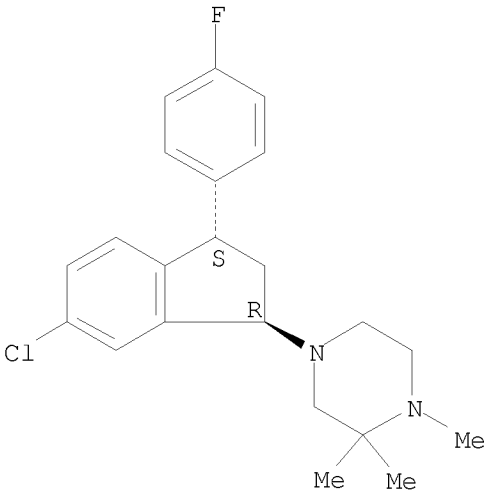
170381-50-7 170381-52-9 170381-54-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as dopamine D1 antagonist)

RN 153626-89-2 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 153626-88-1
CMF C22 H26 Cl F N2

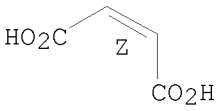
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

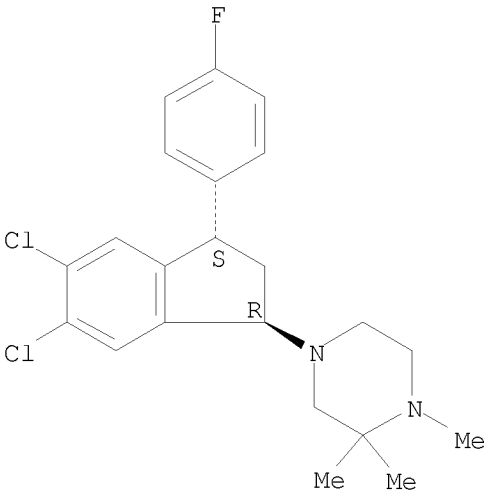


RN 153626-99-4 CAPLUS
CN Piperazine, 4-[(1R,3S)-5,6-dichloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 153626-98-3
CMF C22 H25 Cl2 F N2

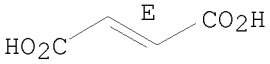
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

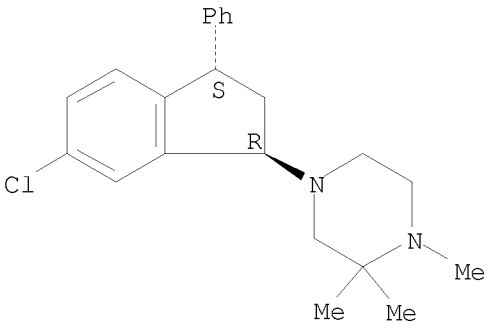


RN 153627-01-1 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-2,3-dihydro-3-phenyl-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 153627-00-0
CMF C22 H27 Cl N2

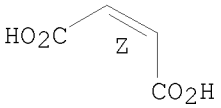
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

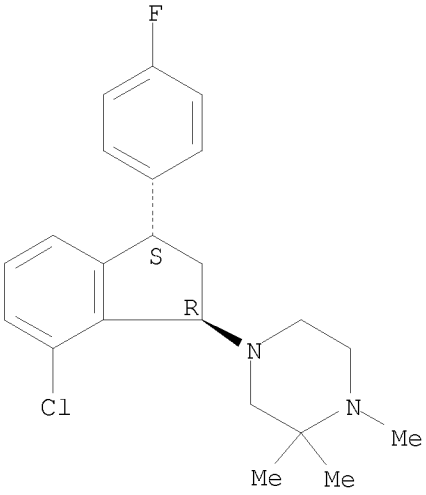


RN 153627-13-5 CAPLUS
CN Piperazine, 4-[7-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (3:4) (9CI) (CA INDEX NAME)

CM 1

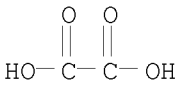
CRN 170381-47-2
CMF C22 H26 Cl F N2

Relative stereochemistry.



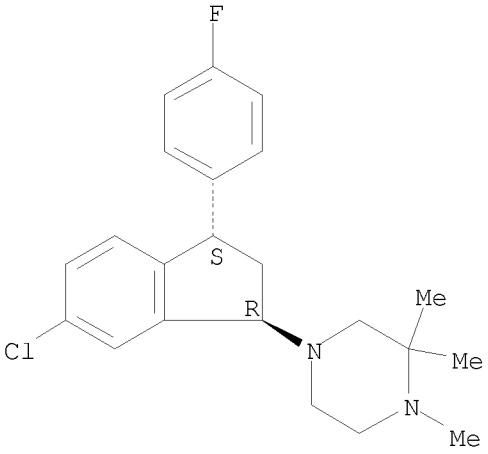
CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 153627-62-4 CAPLUS
CN Piperazine, 4-[6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, dihydrochloride, trans-(-)- (9CI) (CA INDEX NAME)

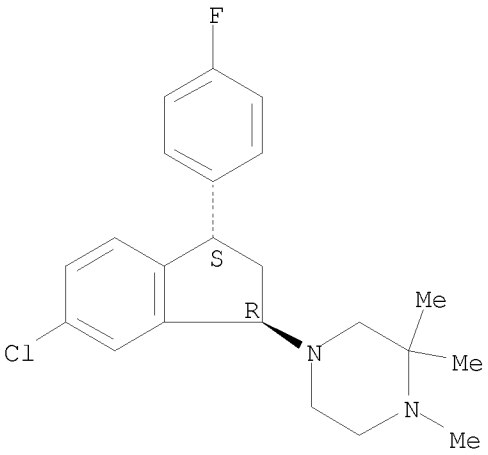
Rotation (-). Absolute stereochemistry unknown.



●2 HCl

RN 153627-64-6 CAPLUS
CN Piperazine, 4-[6-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, dihydrochloride, trans-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



●2 HCl

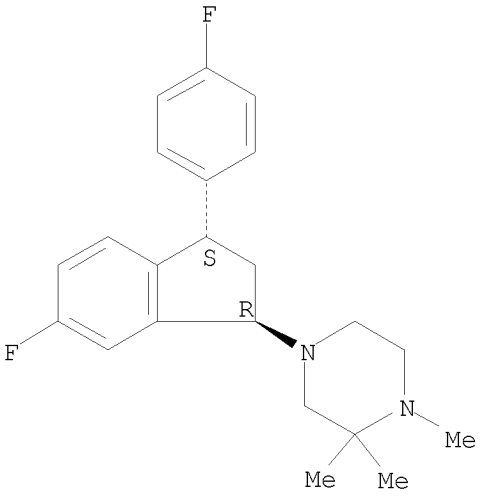
RN 170381-25-6 CAPLUS

CN Piperazine, 4-[(1R,3S)-6-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-24-5
CMF C22 H26 F2 N2

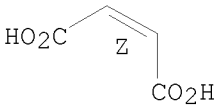
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

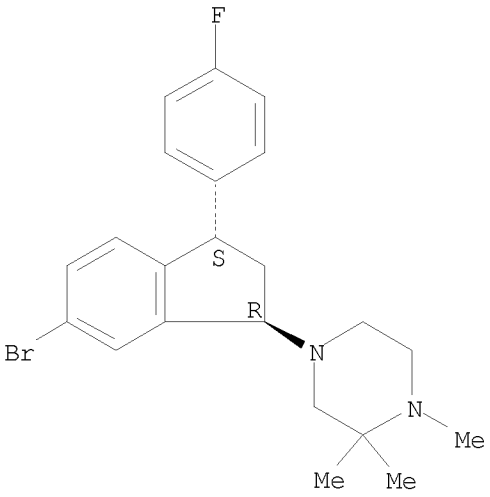


RN 170381-39-2 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-bromo-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-38-1
CMF C22 H26 Br F N2

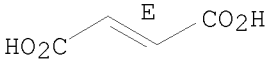
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

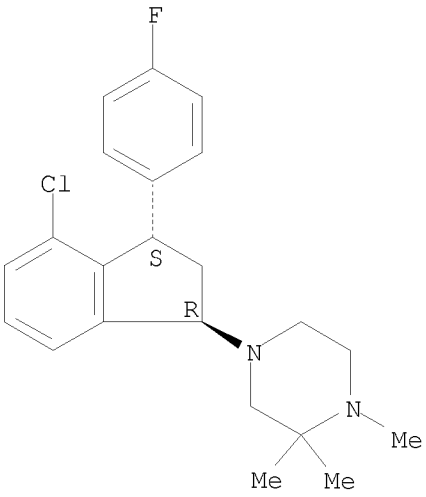


RN 170381-45-0 CAPLUS
CN Piperazine, 4-[4-chloro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:2), trans- (9CI) (CA INDEX NAME)

CM 1

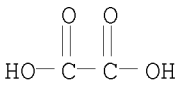
CRN 170381-44-9
CMF C22 H26 Cl F N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

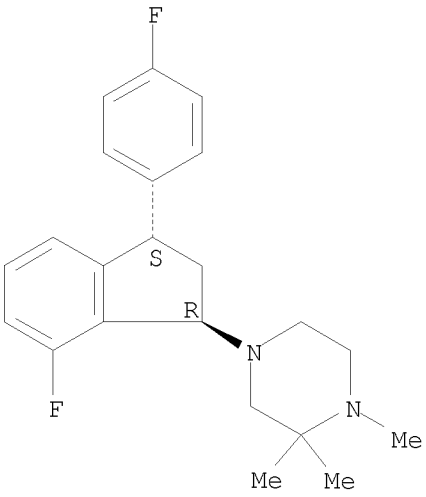


RN 170381-50-7 CAPLUS
CN Piperazine, 4-[7-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, trans-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

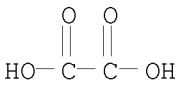
CRN 170381-49-4
CMF C22 H26 F2 N2

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

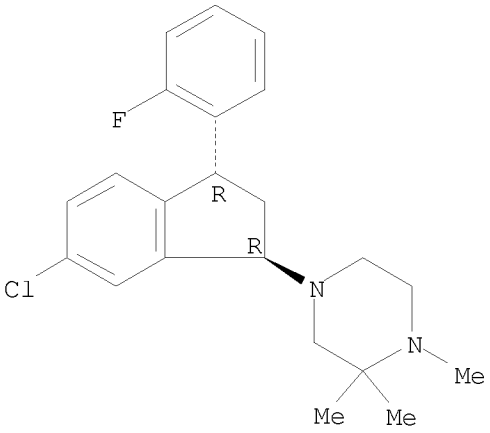


RN 170381-52-9 CAPLUS
CN Piperazine, 4-[(1R,3R)-6-chloro-3-(2-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-51-8
CMF C22 H26 Cl F N2

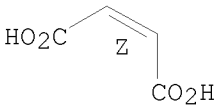
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

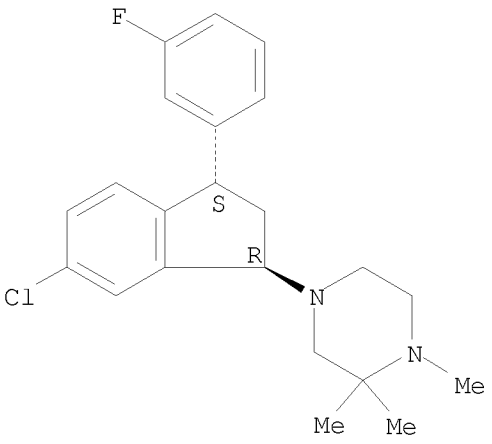


RN 170381-54-1 CAPLUS
CN Piperazine, 4-[(1R,3S)-6-chloro-3-(3-fluorophenyl)-2,3-dihydro-1H-inden-1-yl]-1,2,2-trimethyl-, rel-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 170381-53-0
CMF C22 H26 Cl F N2

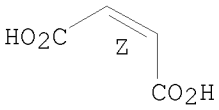
Relative stereochemistry.



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



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L2           43 S L1 SSS FULL
L3           24 S L2 AND NC>1

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L4            4 S L3

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L5            0 L3

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